The Determination of Nuclear Level Densities from Experimental Information

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Abstract

A novel Information Theory based method for determining the density of states from prior information is presented. The energy dependence of the density of states is determined from the observed number of states per energy interval and model calculations suggest that the method is sufficiently reliable to calculate the thermal properties of nuclei over a reasonable temperature range.

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The simplest expression for the nuclear level density has been obtained in the Fermi-gas model by Bethe [1–3] and later modified by Bloch [4–6]. There are, however, a number of shortcomings in this approach. For example, the lack of coupling to the collective part of the nuclear spectrum leads to an energy-independent level density parameter. Recently there has been considerable theoretical activity in the determination of the nuclear many-body density of states, taking into account shell, pairing, and deformation effects [7,8], finite size effects [9], and thermal and quantal effects [10,11] as well as improvements in the determination of the spin cut-off factors [12]. Furthermore, the multiple inverse Laplace transform used to determine the nuclear density of states from the Grand-Canonical partition function of a Fermi gas appears to lead to certain inconsistencies in the folding of nuclear level densities [13]. In spite of these deficiencies Bloch's formula is widely used, particularly as a means of parameterizing the experimentally determined nuclear level densities [14]. Generally the level density parameter is taken to be constant. Should it be energy dependent, an *a priori* form for the energy dependence must be assumed.

In the present work we will demonstrate a simple means of extracting the nuclear level density from the experimental information, based on Information Theory [15]. We wish to determine the distribution of states or level density, $\rho(E)$, for a nucleus such that

$$\int_0^\infty \rho(E)\Theta(E_i - E)\Theta(E - E_{i+1})dE = N_i \quad i = 1, \ldots, N \tag{1}$$

where N_i, the number of states in the energy interval $E_{i+1} - E_i$, is assumed known, and $\Theta(x) = 1$ if $x \geq 0$ and is zero otherwise. As a zeroth-order guess we assume that the distribution of states or level density is given by the Bloch formula

$$\rho_0(E) = \frac{1}{\sqrt{48}E} \exp\left[2\sqrt{a_0 E}\right] \tag{2}$$

where a_0 is the level-density parameter, often expressed in terms of the nuclear mass number A by

$$a_0 = \frac{A}{k_0}, \tag{3}$$

with, for example, $k_0 = 8$ MeV. The actual distribution $\rho(E)$ may now be determined by minimizing the information entropy of $\rho(E)$ relative to $\rho_0(E)$

$$S(\rho, \rho_0) = \int_0^\infty \rho(E) \ln \frac{\rho(E)}{\rho_0(E)} dE \tag{4}$$

subject to the experimental information given in eq. (1). This yields

$$\rho(E) = \rho_0(E) \exp\left[\sum_{i=1}^{N} \lambda_i \Theta(E_i - E)\Theta(E - E_{i+1})\right] \tag{5}$$

where the Lagrange multipliers λ_i for the intervals $E_i \leq E \leq E_{i+1}$ are determined from the experimental information given in eq. (1).

Now suppose we have determined the set of λ_i and we put

$$\lambda(\bar{E}_i) = \lambda_i \tag{6}$$

where $\bar{E}_i$ is the midpoint of the energy interval $E_i \leq E \leq E_{i+1}$. If the $\lambda(\bar{E}_i)$ vary smoothly with energy, a least-squares fit to this quantity should enable us to extrapolate the $\rho(E)$ beyond the region in which the experimental information is known. If this is the case the density of states may now given by

$$\rho(E) = \rho_0(E) e^{-\lambda(E)}, \tag{7}$$

or, from eqs (2) and (3),

$$\rho\left(E\right) = \frac{1}{\sqrt{48}E} \exp\left[2\sqrt{\frac{AE}{k_0}} - \lambda\left(E\right)\right]. \tag{8}$$

Note here that the energy dependence of the density of states is determined from the prior experimental data.

Thermal properties of nuclei are calculated from the nuclear partition function $Z\left(T\right)$ for fixed nuclear mass number A, where T is the nuclear temperature. The contribution to $Z\left(T\right)$ of the continuous part of the nuclear spectrum is

$$Z\left(T\right) = \int_{E_{\min}}^{\infty} \rho\left(E\right) e^{-E/T} dE \tag{9}$$

where $E_{\min}$ is some suitable lower limit.

To test the proposed method we have performed the following model calculations. Rather than use actual experimental information for the number of states N_i in eq. (1), we have generated the N_i by assuming that for energy $E \geq 1$ MeV the experimental distribution of states is given by

$$\rho\left(E\right) = \frac{1}{\sqrt{48}E} \exp\left[2\sqrt{\frac{AE}{k\left(E\right)}}\right] \tag{10}$$

where $k = k(E)$ to allow the energy dependence of the density of states to deviate from the Bloch form. The size of the energy intervals $E_{i+1} - E_i$ in eq. (1) was fixed at 0.4 MeV, with ten such intervals covering the energy range 1–5 MeV. For a particular choice $k(E)$ the Lagrange multipliers λ_i were calculated from eqs (1), (2), (3) and (5), with A arbitrarily set to 56 in eq. (3). A series of least-squares polynomial fits of low order was then performed for the modified Lagrange multipliers

$$\lambda'\left(\bar{E}_i\right) = \frac{\lambda\left(\bar{E}_i\right)}{2\sqrt{AE}}. \tag{11}$$

The many-body density of states and nuclear partition function were then calculated from eqs (8) and (9) , respectively.

A sample fit to $\lambda'\left(\bar{E}_i\right)$ is shown in figure 1 for the choice

$$k(E) = 8 \tag{12}$$

in eq. (10), corresponding to the Bloch formula (2) with $k_0 = 8$; a perfect fit should produce $\lambda' = 0$ identically. Since we take the number of states to be an integer, whereas the integral in (1) with the density of states given by (10) produces a real number, we do not expect to find all the Lagrange multipliers to be zero. The error bars included in the figure were generated by arbitrarily changing the number of states N_i to $N_i \pm \sqrt{N_i/2}$. They serve both to indicate the sensitivity of the calculation to uncertainties in the input, and also to provide a scale for λ'. The fit was also weighted according to these error bars. As figure 1 indicates, the quality of the fit increases as the order of the polynomial is increased, but $\lambda' = 4 \times 10^{-5}$ (constant) is already satisfactory.

The corresponding many-body density of states was calculated from eq. (8) with E extrapolated beyond the region of fit 1–5 MeV to 20 MeV; the density relative to the input density eq. (10) is shown in figure 2. It is seen that $\lambda' =$ constant provides an almost perfect fit for all energies. Polynomial fits of higher order, whilst giving a slightly better fit up to $E = 5$ MeV, cannot be extrapolated much beyond this energy.

The nuclear partition function was computed using eq. (9), with $E_{\min} = 1$ MeV. Due to the rapid increase in the calculated density of states for higher order polynomial fits to the modified Lagrange multipliers, the infinite upper limit of the energy integration was replaced by $E_{\max}$, determined as follows. First, $Z(T)$ for a given temperature was calculated using the input density of states eq. (10), with the upper limit gradually increased until the integral converged to a constant value. The final value for the upper limit, $E_{\max}$, which varied between 30 MeV and 150 MeV depending on T, was then used in the calculation for that temperature with the fitted density of states eq. (8). The results are plotted in figure 3, which shows $Z(T)$ calculated with eq. (8) relative to the partition function calculated with the input density of states. The fit $\lambda' =$ constant produces an almost perfect result up to $T = 2$ MeV, whereas the higher order fits are far from satisfactory except at the lowest temperatures.

These calculations were repeated with other choices for $k(E)$ in eq. (10). For example, the use of

$$k(E) = 6 + E/2 \tag{13}$$

is illustrated in figures 4–6. This choice allows a reasonable energy dependence for the level density parameter, permitting the density of states to deviate sufficiently from the Bloch form to provide a realistic test of the method. (It should be noted that in practice the energy dependence of $k(E)$ is constrained; too strong a dependence causes the density of states to increase rapidly at higher energies or to decrease suddenly to zero.) As seen from figure 4, the lowest order polynomial which fits $\lambda'\left(\bar{E}_i\right)$ within the error bars is linear in energy. Figure 5 shows that this same fit provides a satisfactory description of the density of states

well beyond the energy region in which the fit was produced. The quality of the calculated partition function, shown if figure 6, is excellent.

Finally, we have checked the calculations for sensitivity to various details in the method. For example we have performed calculations in which:

- the energy $\bar{E}_i$ for the energy interval $E_{i+1} - E_i$ was computed as the mean energy weighted according to the density of states, rather than simply as the midpoint energy;
- the fit to $\lambda'\left(\bar{E}_i\right)$ was *not* weighted according to the uncertainty in λ';
- the fit was to $\lambda\left(\bar{E}_i\right)$ rather than to $\lambda'\left(\bar{E}_i\right)$;
- the energy range 1–5 MeV was spanned by 5 intervals of width 0.8 MeV, or 16 intervals of width 0.25 MeV, rather than 10 intervals of width 0.4 MeV.

In most cases the results were not changed significantly. There is a slight preference for fewer, wider energy intervals, and for the fit to λ' to be weighted. A fit to λ', rather than λ, is definitely preferred, at least for those functions $k(E)$ actually used.

A simple Information theory based method for determining the density of states from prior experimental measurements has been presented. A good approximation of the density of states is obtained even at higher energies and any energy dependence is determined from the prior experimental data. However, the extrapolated density of states will not necessarily be very accurate if at higher energies processes occur which are not reflected in the lower energy prior information. With this proviso, the model calculations show that the partition function can be accurately calculated over a reasonable temperature range which suggest that the thermal properties of nuclei can be adequately described by this method.

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FIGURES

FIG. 1. Modified Lagrange multipliers for the case $k(E) = 8$. The circles indicate values computed with eq. (8), the solid line represents the fit with a polynomial of order zero, the dashed line the fit of order one and the dash-dot line the fit of order two. The calculation of the error bars is explained in the text.

FIG. 2. Calculated density of states, relative to the exact density of states, for the case $k(E) = 8$. The solid line is computed with λ fitted with a polynomial of order zero, the dashed line with the fit of order one and the dash-dot line with the fit of order two.

FIG. 3. Calculated partition function, relative to the exact partition function, for the case $k(E) = 8$. The solid line is computed with λ fitted with a polynomial of order zero, the dashed line with the fit of order one and the dash-dot line with the fit of order two.

FIG. 4. Modified Lagrange multipliers for the case $k(E) = 6 + E/2$. The circles indicate values computed with eq. (8), the solid line represents the fit with a polynomial of order zero, the dashed line the fit of order one and the dash-dot line the fit of order two. The calculation of the error bars is explained in the text.

FIG. 5. Calculated density of states, relative to the exact density of states, for the case $k(E) = 6 + E/2$. The solid line is computed with λ fitted with a polynomial of order zero, the dashed line with the fit of order one and the dash-dot line with the fit of order two.

FIG. 6. Calculated partition function, relative to the exact partition function, for the case $k(E) = 6 + E/2$. The solid line is computed with λ fitted with a polynomial of order zero and the dashed line with the fit of order one.

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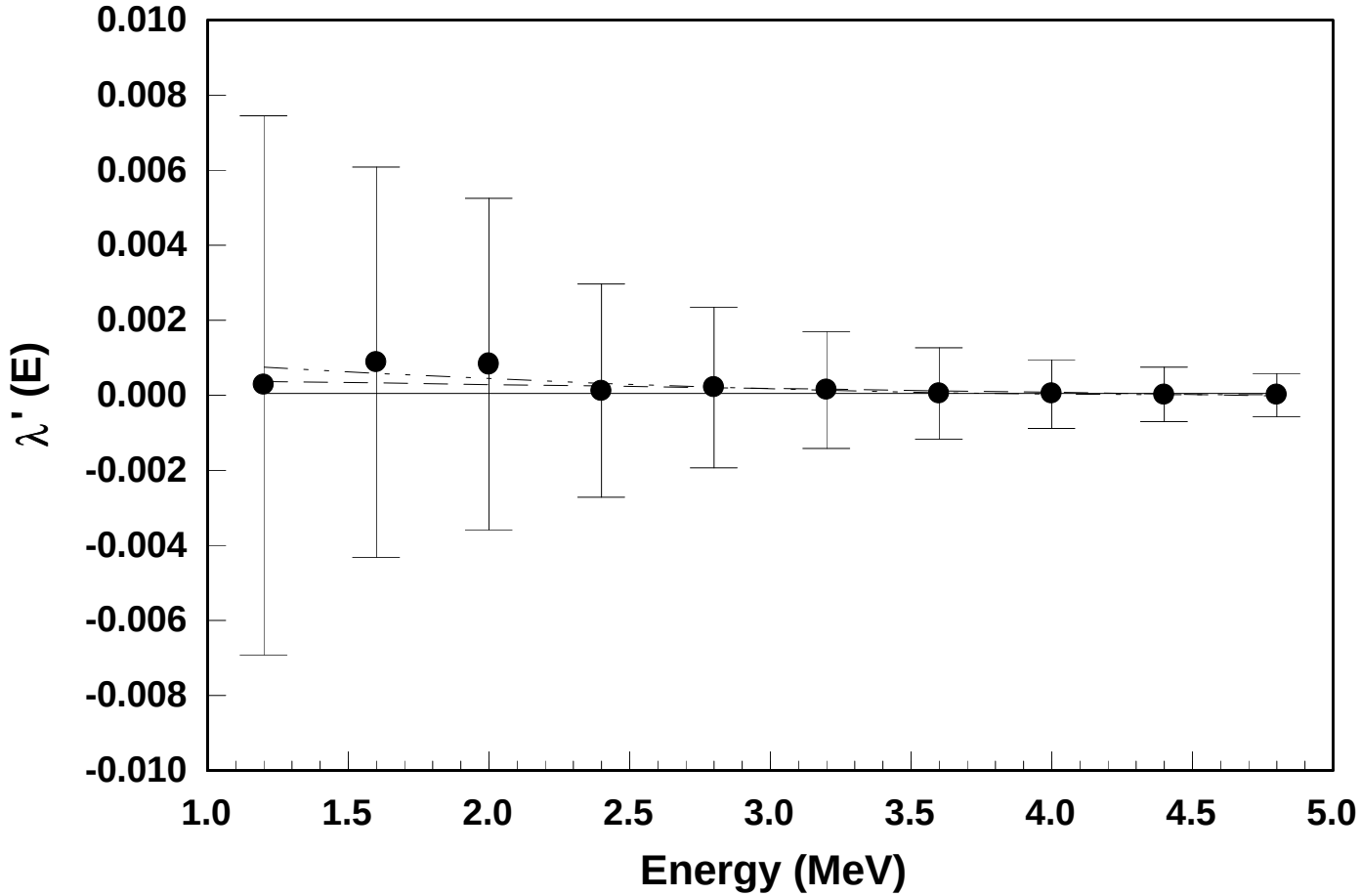
http://arXiv.org/ps/nucl-th/9409001v1


0.010
0.008
0.006
0.004
0.002
0.000
-0.002
-0.004
-0.006
-0.008
-0.010
λ' (E)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Energy (MeV)

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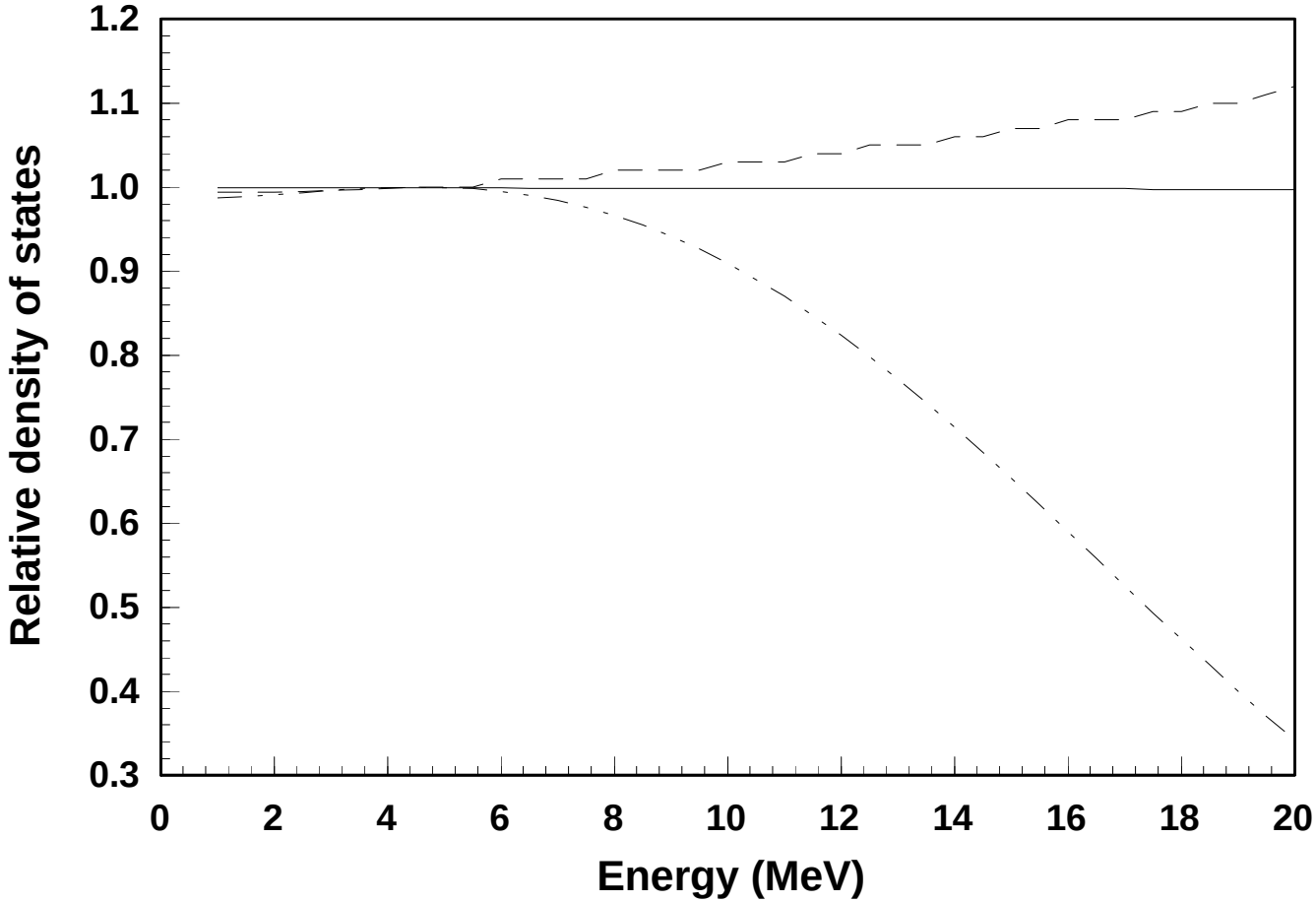
Relative density of states
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0
2
4
6
8
10
12
14
16
18
20
Energy (MeV)

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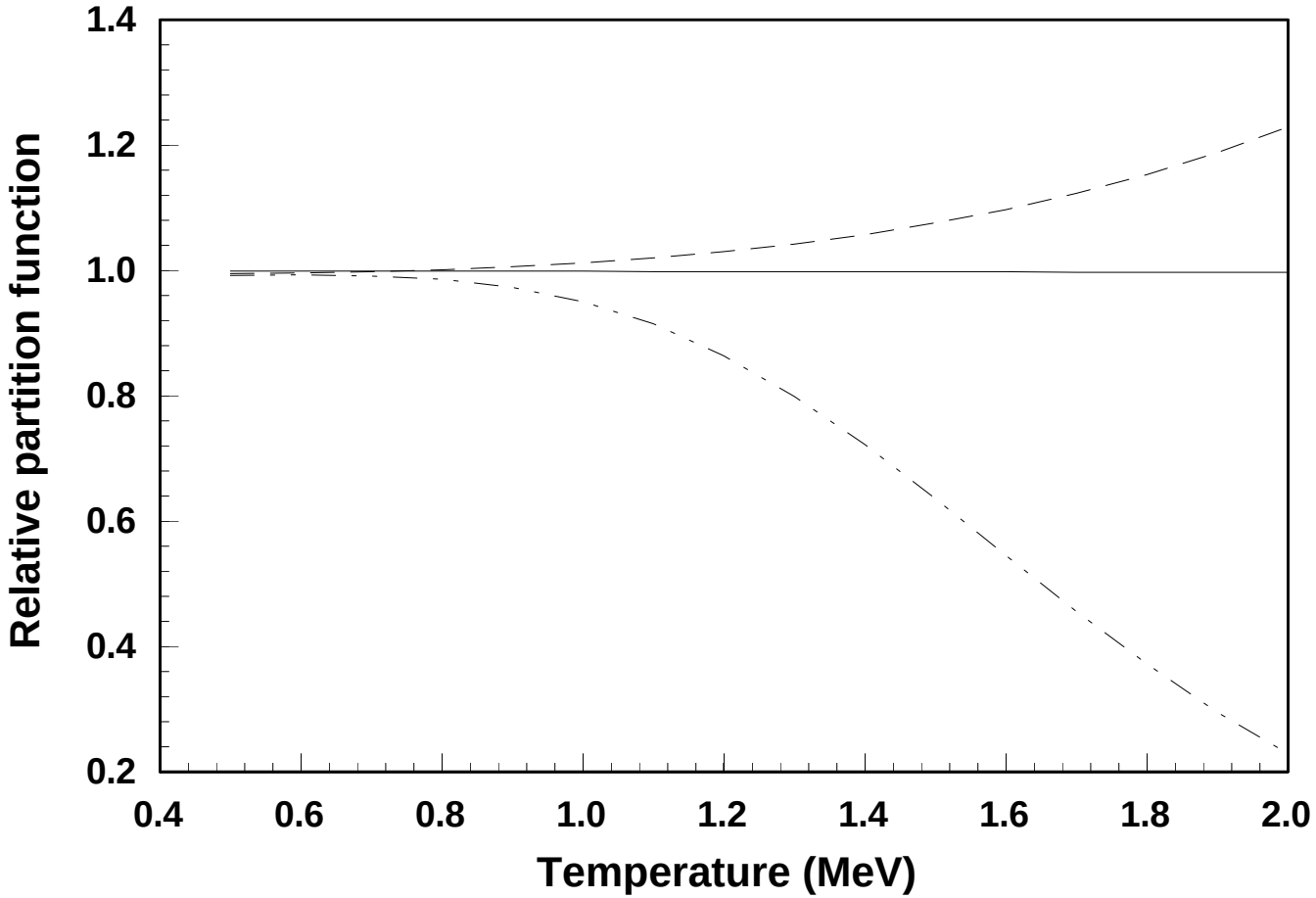
Relative partition function
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Temperature (MeV)

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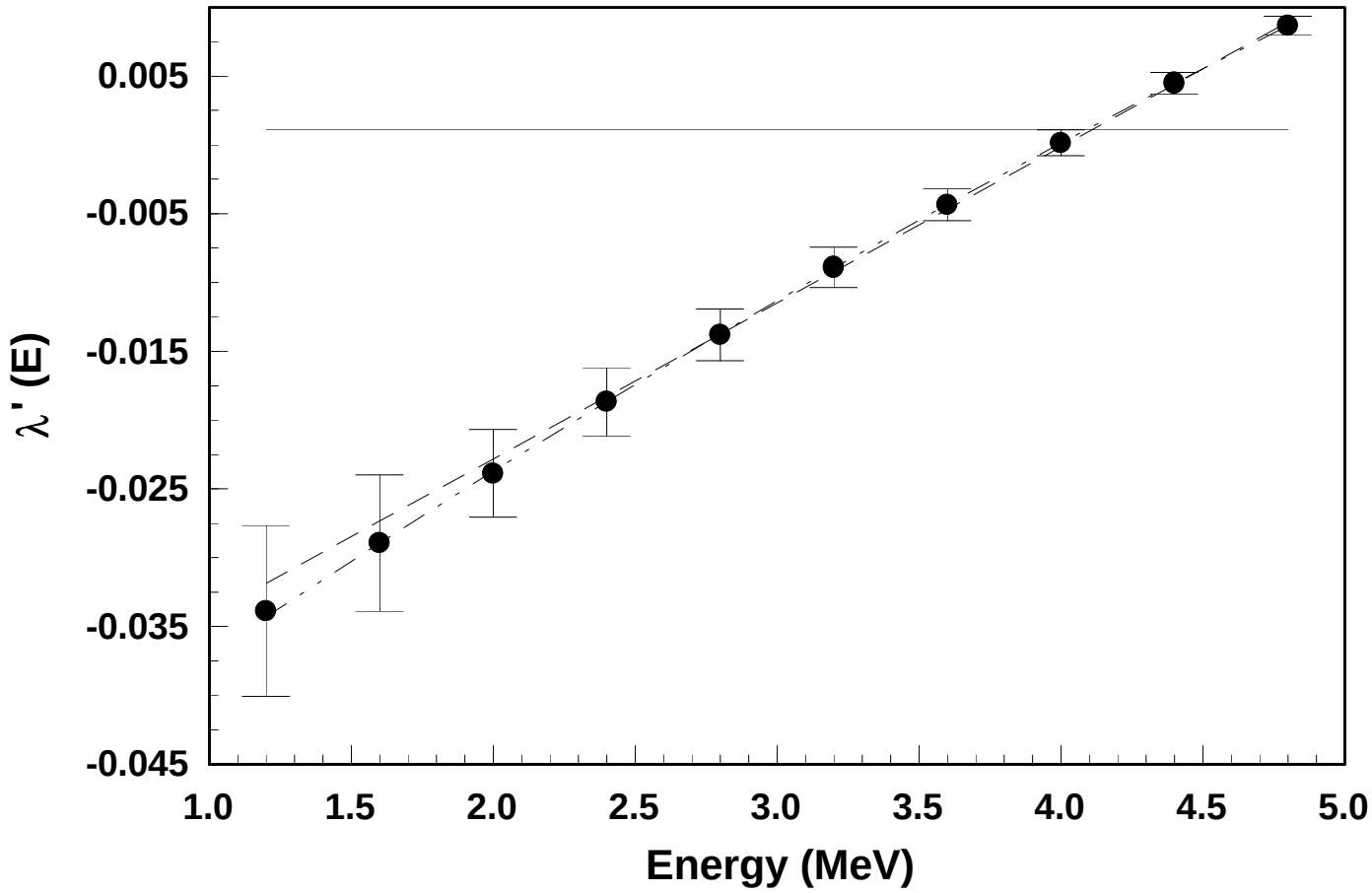
0.005
-0.005
-0.015
-0.025
-0.035
-0.045
λ' (E)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Energy (MeV)

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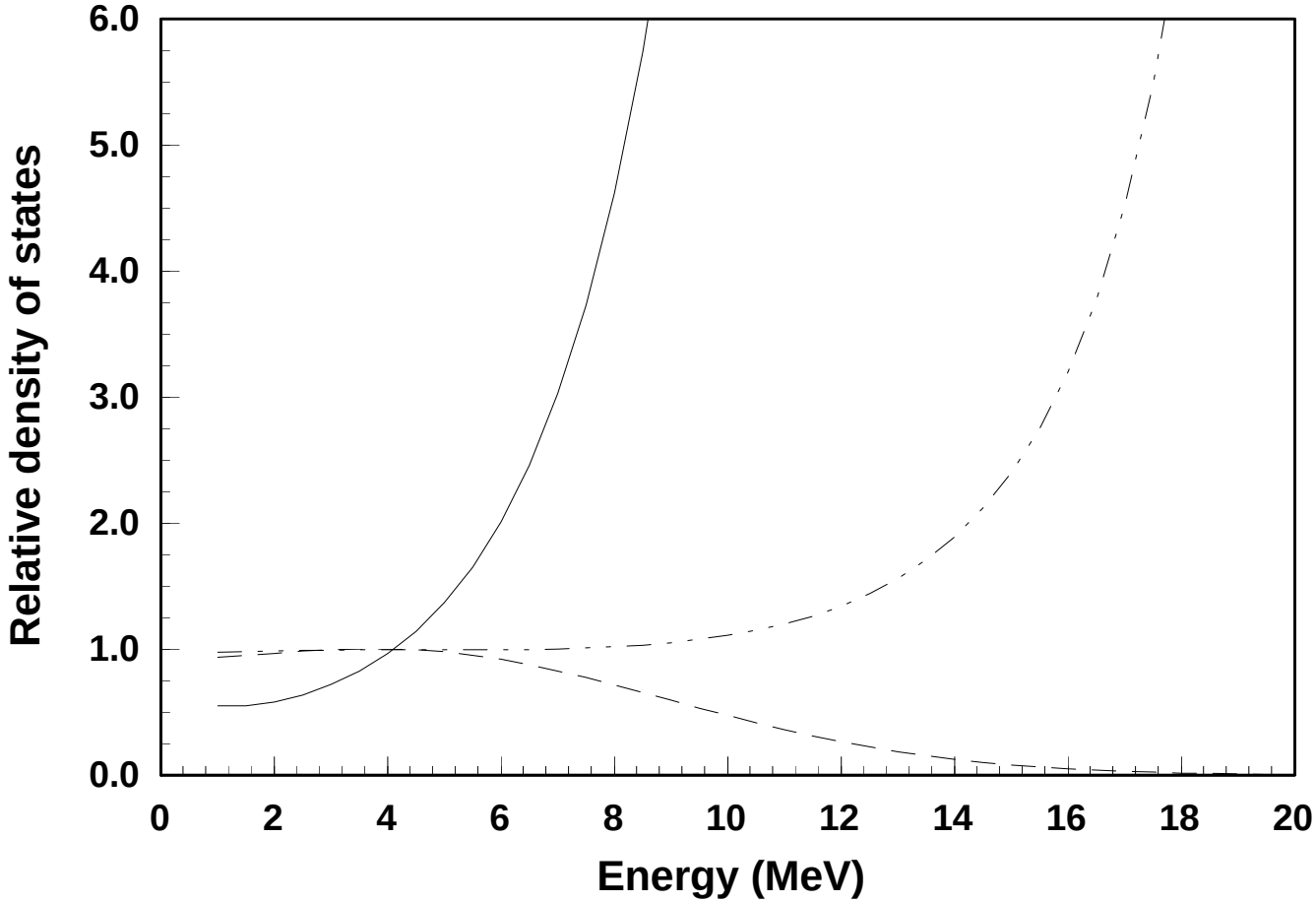
Relative density of states
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0
2
4
6
8
10
12
14
16
18
20
Energy (MeV)

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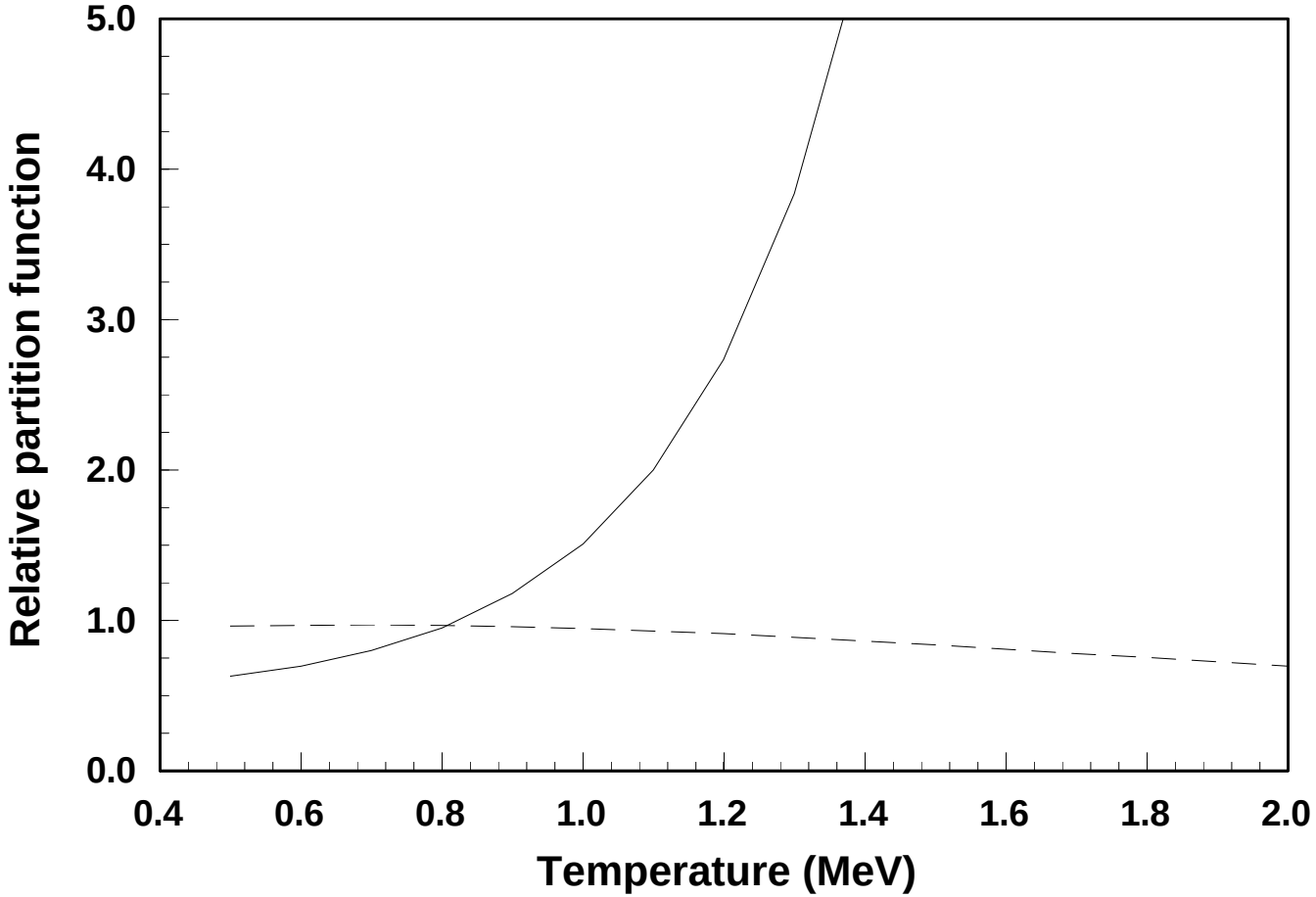
Relative partition function
5.0
4.0
3.0
2.0
1.0
0.0
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Temperature (MeV)